STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 152007

TO: Shailendra Kumar **Location: 5c03 / 5c18** **Monday, May 02, 2005** **Art Unit: 1621** **Phone: 571-272-0640** **Serial Number: 10 / 807206**	**From: Jan Delaval** **Location: Biotech-Chem Library** **Remsen 1a51** **Phone: 571-272-22504** **jan.delaval@uspto.gov**

Search Notes

Jan please

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 4/28/05

Art Unit: 1621 Phone Number: 2-0640 Serial Number: 10/807,206

Location (Bldg/Room#): REM (Mailbox #): 5C18 Results Format Preferred (circle): PAPER /DISK

5C03

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Method of producing an amide.

Inventors (please provide full names): Lawrence Joseph Williams

Earliest Priority Date: 3/23/04

Search Topic:

RU-0195 -33- PATENT

What is claimed is:

1. A method for producing an amide comprising combining a thio acid and an organic azide in the presence of a solvent so that an amide is produced.

APR 28 2005 (STIC)

****

STAFF USE ONLY

Searcher: am

Searcher Phone #: 22504

Searcher Location:

Date Searcher Picked Up: 5/2/05

Date Completed: 5/2/05

Searcher Prep & Review Time: 20

Online Time: +40

Type of Search

___ NA Sequence (#)

___ AA Sequence (#)

✓ Structure (#) 3

___ Bibliographic

___ Litigation

___ Fulltext

___ Other

Vendors and cost where applicable

✓ STN ___ Dialog

___ Questel/Orbit ___ Lexis/Nexis

___ Westlaw ___ WWW/Internet

___ In-house sequence systems

___ Commercial ___ Oligomer ___ Score/Length

___ Interference ___ SPDI ___ Encode/Transl

___ Other (specify)

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=> fil casreact
FILE 'CASREACT' ENTERED AT 09:29:39 ON 02 MAY 2005
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FILE CONTENT:1840 - 1 May 2005 VOL 142 ISS 18

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************************************************************
*                                                          *
*     CASREACT now has more than 9.2 million reactions     *
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d his

     (FILE 'HOME' ENTERED AT 08:56:08 ON 02 MAY 2005)
               SET COST OFF

     FILE 'CASREACT' ENTERED AT 08:56:16 ON 02 MAY 2005
               E AZIDE/FG.RCT
               E AZIDE/FG.RGT
L1          8809 S AZIDE/FG.RCT,FG.RGT
               E AMIDE/FG.PRO
L2          3584 S E3 AND L1
L3            21 S L2 AND (THIO OR THIOACETIC OR THIOBENZOIC)()ACID
L4            16 S L2 AND (THIOACETATE OR THIOBENZOATE)
L5            34 S L3,L4

     FILE 'REGISTRY' ENTERED AT 08:58:34 ON 02 MAY 2005
L6             1 S THIOACETIC ACID/CN
L7             1 S THIOBENZOIC ACID/CN
L8            86 S 507-09-5/CRN
L9            69 S 98-91-9/CRN
L10          109 S L8,L9 NOT (MNS OR MXS OR CCS OR PMS OR IDS)/CI
L11           23 S L10 NOT SALT
L12           86 S L10 NOT L11

     FILE 'HCAPLUS' ENTERED AT 09:00:49 ON 02 MAY 2005

     FILE 'CASREACT' ENTERED AT 09:01:13 ON 02 MAY 2005
L13           82 S L2 AND L6
L14            4 S L2 AND L7
L15           28 S L2 AND L12
L16          115 S L5,L13-L15
L17           67 S L2 AND L6/RCT
L18           15 S L2 AND L6/RGT
L19            4 S L2 AND L7/RCT
L20            0 S L2 AND L7/RGT
L21           25 S L2 AND L12/RCT
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L22           6 S L2 AND L12/RGT
L23         109 S L17-L22
L24           6 S L16 NOT L23

     FILE 'REGISTRY' ENTERED AT 09:04:10 ON 02 MAY 2005
L25           1 S METHANOL/CN

     FILE 'HCAPLUS' ENTERED AT 09:04:13 ON 02 MAY 2005

     FILE 'CASREACT' ENTERED AT 09:04:16 ON 02 MAY 2005
L26          92 S L25 AND L23
L27           8 S (MEOH OR METHANOL OR METHYLALCOHOL OR METHYL ALCOHOL) AND L23
L28          93 S L26,L27
L29          16 S L23 NOT L28
                SEL DN AN 5 7 12
L30           3 S L29 AND E1-E6
L31          18 S L28 AND (BENZYL PROTECTED GLYCAN OR NAPHTHYRIDINE OR ASYMMETR
L32           8 S L28 AND (CHEMOSELECTIVE OR MACROBICYCLID OR DESIGN OR THIO AC
L33          25 S L31,L32
L34          10 S L33 AND (GEMINI OR XXIV OR 6 SULFATE OR SPACER OR O LINKED OR
L35          15 S L33 NOT L34
L36          14 S L35 NOT KHAFREFUNGIN/TI
L37           1 S L28 AND MACROBICYCLIC/TI
L38          15 S L36,L37
                E WILLIAMS L/AU
L39          10 S E3,E6,E9
L40           1 S L39 AND L2
L41          15 S L38,L40
L42           9 S L39 NOT L41
L43           1 S L39 AND L1
L44           4 S L39 AND AMIDE/FG.PRO
L45           3 S L43,L44 NOT L41
L46           0 S L45 AND L6,L7,L12
L47           0 S L45 AND THIO?

     FILE 'CASREACT' ENTERED AT 09:29:39 ON 02 MAY 2005

=> d bib abs fhit retable tot l41


L41  ANSWER 1 OF 15  CASREACT  COPYRIGHT 2005 ACS on STN
AN   141:89339  CASREACT
TI   An o-nitrobenzyl scaffold for peptide ligation:
     synthesis and applications
AU   Marinzi, Chiara; Offer, John; Longhi, Renato; Dawson, Philip E.
CS   C. N. R., Istituto di Chimica del Riconoscimento Molecolare, Milan, 20131,
     Italy
SO   Bioorganic & Medicinal Chemistry (2004), 12(10), 2749-2757
     CODEN: BMECEP; ISSN: 0968-0896
PB   Elsevier Ltd.
DT   Journal
LA   English
AB   Chemical ligation approaches facilitate the chemoselective assembly of
     unprotected peptides in aqueous solution Here, two photolabile auxiliaries are
     described that enlarge the applicability of native chemical ligation to
     non-cysteine targets.  The auxiliaries, designed to allow reaction with
     thioester peptides, generate an amide bond between the two initial
     fragments.  The o-nitrobenzyl tertiary benzylamide that is formed at the
     ligation junction can be transformed into a native amide group under mild
     photolysis conditions.  The veratryl auxiliary was found to be excessively
     labile during peptide purification and ligation.  However, the auxiliary based
     on the o-nitrobenzyl group shows all the necessary properties for a
     general application in routine peptide and protein synthesis.  In addition,
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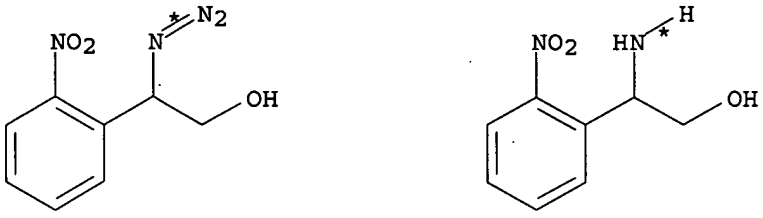
the auxiliary linked to the N-terminus can be efficiently photolyzed, suggesting a new approach for the generation of photocaged amines. Synthesis, solid phase introduction onto peptide chains, ligation properties and photolysis in water are described, and a careful study of compatibility of the method with potentially fragile peptide side chains is reported.

RX(3) OF 58 ...**F** ===> I...



F I
YIELD 91%

RX(3) RCT F **716345-77-6**
RGT J 603-35-0 PPh3
PRO I 716345-79-8
SOL 7732-18-5 Water, 109-99-9 THF

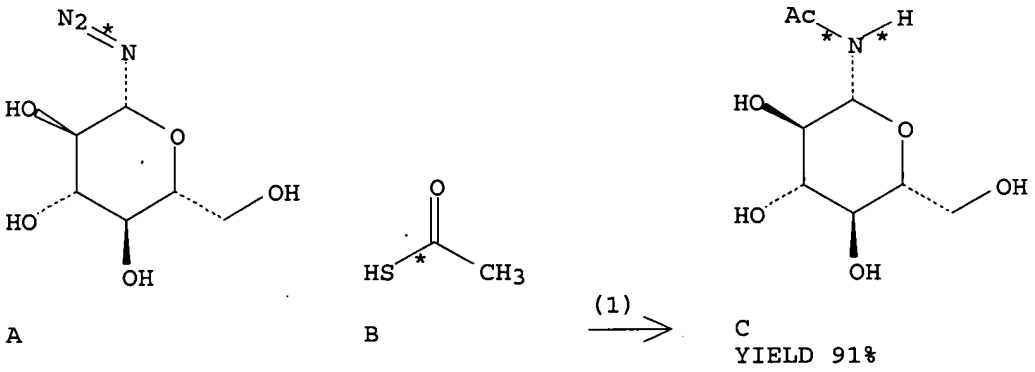
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Ajayaghosh, A	1995	36	777	Tetrahedron Lett	CAPLUS
Atherton, E	1990		11	Innovation Perspect	CAPLUS
Atherton, E	1987	9	1	The Peptides	CAPLUS
Bochet, C	2002		125	J Chem Soc, Perkin T	CAPLUS
Bosques, C	2003	125	7530	J Am Chem Soc	CAPLUS
Botti, P	2001	42	1831	Tetrahedron Lett	CAPLUS
Bruice, T	1964	86	4886	J Am Chem Soc	CAPLUS
Caldon, M	1988	4	99	Proteins	
Canne, L	1996	118	5891	J Am Chem Soc	CAPLUS
Dawson, P	2000	69	923	Ann Rev Biochem	CAPLUS
Dawson, P	1994	226	776	Science	
Ellis-Davies, K	1994	91	187	Proc Acad Natl Sci U	
Guiller, F	2000	100	2019	Chem Rev	
Hackeng, T	1999	96	10068	Proc Natl Acad Sci U	CAPLUS
Hasan, A	1997	53	4247	Tetrahedron	CAPLUS
Holmes, C	1997	62	2370	J Org Chem	CAPLUS
Kalbag, S	1975	97	440	J Am Chem Soc	CAPLUS
Kawakami, T	2001	3	1403	Org Lett	CAPLUS
Kawakami, T	2003	44	6059	Tetrahedron Lett	CAPLUS
Kent, S	1992		1	Second International	CAPLUS
Marinzi, C	2001	9	2323	Biorg Med Chem	CAPLUS
Miknis, G	1993	115	536	J Am Chem Soc	CAPLUS
Mintz, M	1983	V	183	Org Synth	
Muir, T	2003	72	249	Ann Rev Biochem	CAPLUS
Nicolau, K	1997	119	449	J Am Chem Soc	
Offer, J	2002	124	4642	J Am Chem Soc	CAPLUS
Offer, J	2000	2	23	Org Lett	CAPLUS
Patchornik, A	1972	37	2281	J Org Chem	
Pillai, V	1987	9	225	Org Photochem	
Pillai, V	1980		1	Synthesis	CAPLUS
Reddy, K	1998	120	1207	J Am Chem Soc	CAPLUS

Rozwadowska, M	1997	53	10615	Tetrahedron	CAPLUS
Sarin, V	1981	117	147	Anal Biochem	CAPLUS
Schnolzer, M	1992	40	180	Int J Pept Protein R	MEDLINE
Tatsu, Y	2002	525	20	FEBS Lett	CAPLUS
Vizzavona, J	2002	12	1963	Biorg Med Chem Lett	CAPLUS
Voelker, T	1998	39	359	Tetrahedron Lett	CAPLUS
Walker, J	1988	110	7170	J Am Chem Soc	CAPLUS
Xiong, C	2002	67	1399	J Org Chem	CAPLUS
Xiong, C	2002	67	3515	J Org Chem	
Zuckermann, R	1992	114	10646	J Am Chem Soc	CAPLUS

L41 ANSWER 2 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 140:128580 CASREACT
TI **RuCl3**-promoted amide formation from azides and **thio-acids**
AU Fazio, Fabio; Wong, Chi-Huey
CS Department of Chemistry and Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Tetrahedron Letters (2003), 44(51), 9083-9085
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science B.V.
DT Journal
LA English
AB Described here is the Ru(III)-promoted amide formation from sugar azides and thio-acids, (e.g., thiolacetic acid) which were shown not to form amides at room temperature in the absence of ruthenium. We believe that a complex formed by Ru(III) increases the reactivity of the thiocarbonyl species and therefore reaction with azides occurs at room temperature, even when
less reactive (electron rich and/or sterically hindered) azides are employed.

RX(1) OF 7 **A** + **B** ===> **C**



RX(1) RCT A **20379-59-3**, B **507-09-5**
RGT D 108-48-5 2,6-Lutidine
PRO C **6983-36-4**
CAT 10049-08-8 RuCl3
SOL **67-56-1** MeOH
NTE yield depends on amt. of cat.

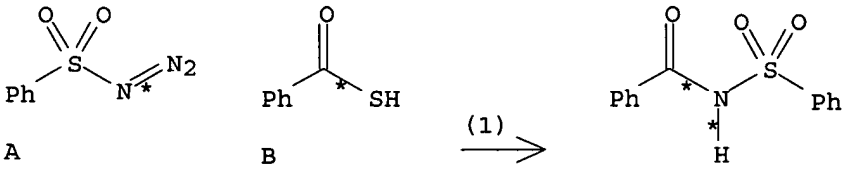
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File

Alper, P	1996	37	6029	Tetrahedron Lett	CAPLUS
Brik, A	2002	9	891	Chem Biol	CAPLUS
Fazio, F	2002	124	14397	J Am Chem Soc	CAPLUS
Gothelf, K	1998	98	863	Chem Rev	CAPLUS
Nyffeler, P	2002	124	10773	J Am Chem Soc	CAPLUS
Rosen, T	1988	53	1580	J Org Chem	CAPLUS
Rostovtsev, V	2002	41	2596	Angew Chem, Int Ed	CAPLUS
Schenk, W	2002	661	129	J Organomet Chem	CAPLUS
Shangguan, N	2003	125	7754	J Am Chem Soc	CAPLUS
Tornoe, C	2002	67	3057	J Org Chem	CAPLUS

L41 ANSWER 3 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 139:213881 CASREACT
TI The Reaction of **Thio Acids** with Azides: A New Mechanism and New Synthetic Applications
AU Shangguan, Ning; Katukojvala, Sreenivas; Greenberg, Rachel; **Williams, Lawrence J.**
CS Department of Chemistry and Chemical Biology, Rutgers The State University of New Jersey, Piscataway, NJ, 08854, USA
SO Journal of the American Chemical Society (2003), 125(26), 7754-7755
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB A new amide synthesis strategy based on a fundamental mechanistic revision of the reaction of thio acids and organic azides is presented. It was shown that amines are not formed as intermediates in this reaction, and alternative mechanisms proceeding through a thiatriazoline intermediate are suggested. The reaction has been applied to the preparation of both simple and architecturally complex amides that are difficult to access using conventional methods. The reaction is chemoselective, effective for unprotected substrates, and compatible with aprotic and protic solvents, including water.

RX(1) OF 30 A + **B** ===> **C**



A B C

YIELD 98%

RX(1) RCT A 938-10-3, B **98-91-9**
RGT D 108-48-5 2,6-Lutidine
PRO C **3559-04-4**
SOL **67-56-1** MeOH

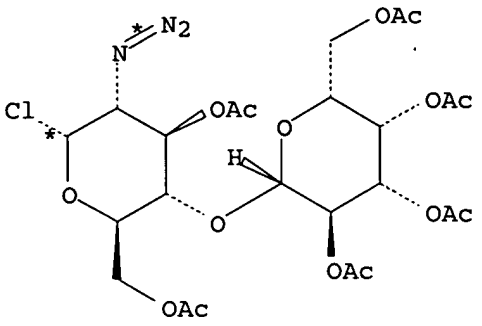
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Backes, B	1999	64	2322	J Org Chem	CAPLUS
Beligere, G	2000	122	12079	J Am Chem Soc	CAPLUS
Canne, L	1995	36	1217	Tetrahedron Lett	CAPLUS
Chin, J	2002	124	9026	J Am Chem Soc	CAPLUS
Chou, S	1997		1691	J Chem Soc, Perkin T	CAPLUS

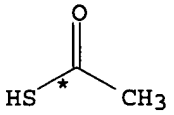
Cohen-Anisfeld, S	1993	115	10531	J Am Chem Soc	CAPLUS
Cornish, V	1995	34	621	Angew Chem, Int Ed E	CAPLUS
Damkaci, F	2003	125		J Am Chem Soc	CAPLUS
Elofsson, M	1997	53	369	Tetrahedron	CAPLUS
Goldstein, A	2000	41	2797	Tetrahedron Lett	CAPLUS
Hakimelahi, G	1980	21	2119	Tetrahedron Lett	CAPLUS
Humphrey, J	1997	97	2243	Chem Rev	CAPLUS
Loock, E	1973	38	2916	J Org Chem	
L'Abbe, G	1980	19	276	Angew Chem, Int Ed E	
L'Abbe, G	1990	27	1059	J Heterocycl Chem	CAPLUS
L'Abbe, G	1975	40	1728	J Org Chem	CAPLUS
Marcaurelle, L	2001	123	1587	J Am Chem Soc	CAPLUS
McKervey, M	1993		94	J Chem Soc, Chem Com	CAPLUS
Nilsson, B	2001	3	9	Org Lett	CAPLUS
Nilsson, W	2000	2	1939	Org Lett	
Offer, J	2002	124	4642	J Am Chem Soc	CAPLUS
Offer, J	2000	2	23	Org Lett	CAPLUS
Park, S	2002	43	6309	Tetrahedron Lett	CAPLUS
Paulsen, H	1994		369	Liebigs Ann Chem	CAPLUS
Rajagopalan, S	1997	27	187	Synth Commun	CAPLUS
Rakotomanomana, N	1990	197	318	Carbohydr Res	CAPLUS
Rijkers, D	2002	43	3657	Tetrahedron Lett	CAPLUS
Rosen, T	1988	53	1580	J Org Chem	CAPLUS
Saxon, E	2000	2	2141	Org Lett	CAPLUS
Saxon, E	2000	287	2007	Science	CAPLUS
Schwabacher, A	1993	34	1269	Tetrahedron Lett	CAPLUS
Scriven, E	1988	88	297	Chem Rev	CAPLUS
Suh, E	1994	116	11205	J Am Chem Soc	CAPLUS
Tam, J	2001	60	194	Biopolymers	CAPLUS
Tamura, M	1984	57	3167	Bull Chem Soc Jpn	CAPLUS

L41 ANSWER 4 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 139:180265 CASREACT
TI Synthesis of a useful anomeric **thioacetate** of an N-acetyllactosamine derivative and its application
AU Matsuoka, Koji; Ohtawa, Takumi; Hinou, Hiroshi; Koyama, Tetsuo; Esumi, Yasuaki; Nishimura, Shin-Ichiro; Hatano, Ken; Terunuma, Daiyo
CS Faculty of Engineering, Department of Functional Materials Science, Saitama University, Saitama, 338-8570, Japan
SO Tetrahedron Letters (2003), 44(18), 3617-3620
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
AB A novel anomeric β-thioacetate of an N-acetyllactosamine derivative was efficiently synthesized in high yield from the known 2-azido glycosyl chloride using thioacetic acid as a convenient reagent. The synthesis involved not only an SN2 replacement of the chloride by a carbothiolate anion but also a reductive acetamidation of the azide group. Applications of the thioacetate for glycosidation were demonstrated to provide both O- and S-glycosides in high yields. Furthermore, both intermediates gave a new class of glycoclusters that included thioglycosidic linkages.

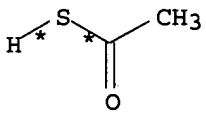
RX(1) OF 20 **A** + 2 **B** ===> **C**...



A

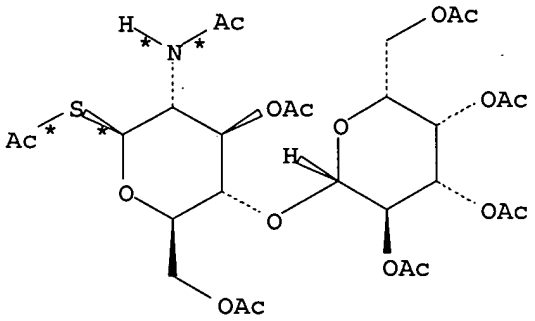


B



B

(1) ⟶



C

RX(1) RCT A **68733-23-3**, B **507-09-5**
PRO C **577993-52-3**
SOL 110-86-1 Pyridine

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Ball, E	1992	114	5449	J Am Chem Soc	
Bielfeldt, T	1992		857	Angew Chem, Int Ed E	
Chen, X	1998	120	7760	J Am Chem Soc	CAPLUS
Fukuda, M	1993			Glycobiology	
Garegg, P	1997	52	179	Adv Carbohydr Chem B	CAPLUS
Hasegawa, A	1986	5	11	J Carbohydr Chem	CAPLUS
Kameyama, A	1991	209	c1	Carbohydr Res	CAPLUS
Lemieux, R	1979	57	1244	Can J Chem	CAPLUS
Matsuoka, K	1998	71	2709	Bull Chem Soc Jpn	CAPLUS
Matsuoka, K	2000	329	765	Carbohydr Res	CAPLUS
Matsuoka, K	2000	57	691	Kobunshironbunsyu	CAPLUS
Matsuoka, K	1999	40	7839	Tetrahedron Lett	CAPLUS
Matsuoka, K	2001	42	3327	Tetrahedron Lett	CAPLUS
Nakahara, Y	1996	292	71	Carbohydr Res	CAPLUS
Nicolaou, K	1990	112	3693	J Am Chem Soc	CAPLUS
Nicolaou, K	1991		870	J Chem Soc, Chem Com	CAPLUS
Nishimura, S	1992		1413	Chem Lett	CAPLUS
Nishimura, S	1991	24	4236	Macromolecules	CAPLUS
Rosen, T	1988	53	1580	J Org Chem	CAPLUS
Terunuma, D	1998		59	Chem Lett	CAPLUS
Yoshino, T	1992	9	287	Glycoconjugate J	

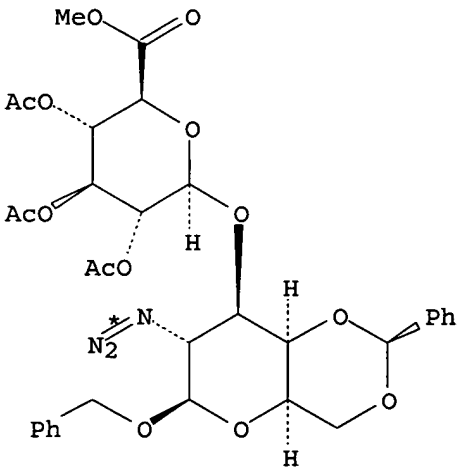
L41 ANSWER 5 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 139:178818 CASREACT
TI Enzymic manufacture of **chondroitin** and derivatives
IN Kobayashi, Shiro; Ohmae, Masashi
PA Denki Kagaku Kogyo Kabushiki Kaisha, Japan
SO PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003070960	A1	20030828	WO 2002-JP11576	20021106

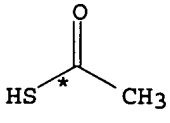
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI JP 2002-42907 20020220
AB The chondroitin (I) is manufactured from an oxazoline derivative with hyaluronic acid-degrading enzyme such as mammalian hyaluronidase. I and its derivs. are useful for manufacturing cosmetics, pharmaceuticals, medical goods, etc. Preparation of a chondrosin oxazoline derivative, polymerization of the oxazoline derivative with ovine testicle hyaluronidase to manufacture I were shown. Also given was chemical synthesis of several chondroitin derivs.

RX(1) OF 59 ...**A** + **B** ===> **C**...

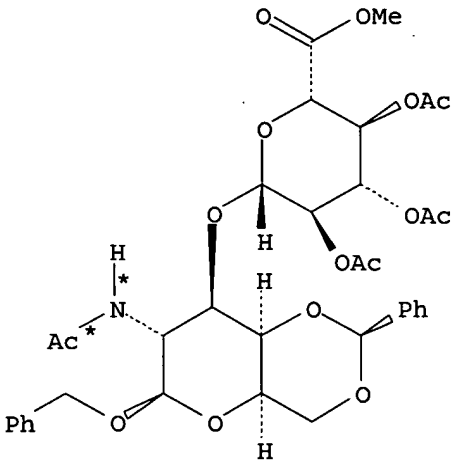


A



B

(1) →



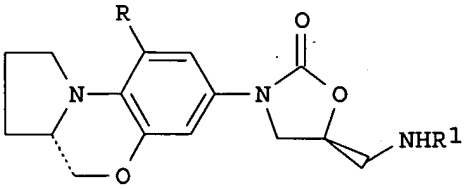
C
YIELD 86%

RX(1) RCT A **581814-26-8**, B **507-09-5**
PRO C **581814-27-9**

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Kobayashi, S	1996	118	13113	J Am Chem Soc	CAPLUS
Kobayashi, S	2001	123	11825	J Am Chem Soc	CAPLUS
Kobayashi, S	1998	132	415	Macromol Symp	
Kobayashi, S	2002	51	901	Polymer Preprints	
Kobayashi, S	2002		817	Sen'i Jotai Analogue	
Shin-Etsu Chemical Co L	1997			JP 09-3088 A	CAPLUS
Takagaki, K	2000	12	295	Trends in Glycoscien	CAPLUS

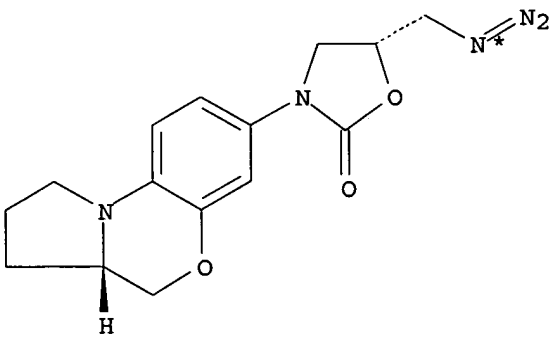
L41 ANSWER 6 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 137:262976 CASREACT
TI Synthesis of Conformationally Constrained Analogs of **Linezolid**: Structure-Activity Relationship (SAR) Studies on Selected Novel Tricyclic Oxazolidinones
AU Selvakumar, Natesan; Srinivas, Deekonda; Khera, Manoj Kumar; Kumar, Magadi Sitaram; Mamidi, Rao N. V. S.; Sarnaik, Hemanth; Charavaryamath, Chandrashekar; Rao, Bonthu Srinivasa; Raheem, Mohammed A.; Das, Jagattaran; Iqbal, Javed; Rajagopalan, Ramanujam
CS Anti-Infectives Discovery Group, Dr. Reddy's Research Foundation, Hyderabad, 500 050, India
SO Journal of Medicinal Chemistry (2002), 45(18), 3953-3962
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



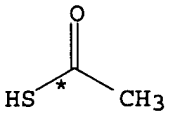
I

AB In an effort to discover potent antibacterials based on the entropically favored "bioactive conformation" approach, we have designed and synthesized a series of novel tricyclic mols. mimicking the conformationally constrained structure of the oxazolidinone antibacterial Linezolid. Structure I (R = H, R1 = Ac), obtained by this approach, was synthesized and found to be moderately active against a panel of Gram-pos. organisms. Further introduction of a fluorine atom in the aromatic ring of this compound, as in Linezolid, resulted in some excellent compds. possessing potent antibacterial activity. The thus obtained lead mol. I (R = F, R1 = Ac) was further fine-tuned by structure-activity relationship studies on the amide functionality leading to a number of novel tricyclic oxazolidinone derivs. Some particularly interesting compds. include the thioamides I (R = F; R1 = CSMe, CSEt), thiocarbamate I (R = F, R1 = CSOMe), and thiourea I (R = F, R1 = CSNH2). The in vitro activity results of amide homologs of I (R = F, R1 = Ac) revealed that compds. up to four carbon atoms on the amide nitrogen retain the activity. In general, thioamides and thiocarbamates are more potent when compared to the corresponding amides and carbamates.

RX(1) OF 402 ...**A** + **B** ===> **C**

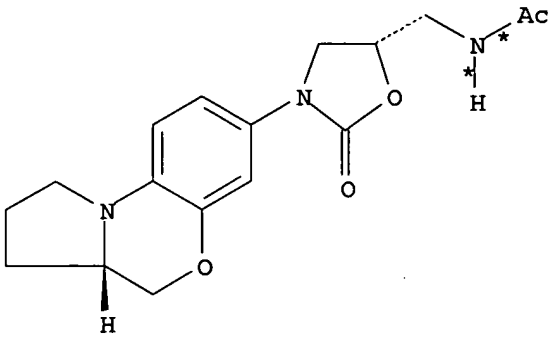


A



B

(1) →



C
YIELD 63%

RX(1) RCT A **463361-54-8**, B **507-09-5**
PRO C **463361-50-4**
SOL 507-09-5 AcSH

RETABLE

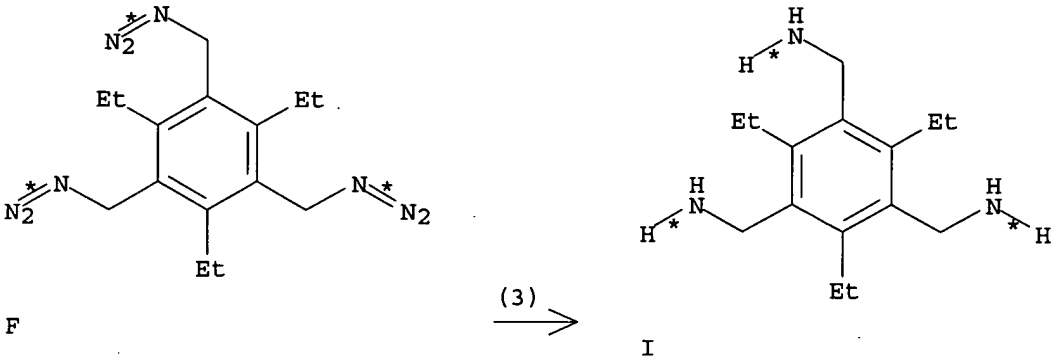
Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Barbachyn, M	1996	39	680	J Med Chem	CAPLUS
Brickner, S	1996	2	175	Curr Pharm Des	CAPLUS
Brickner, S	1996	39	673	J Med Chem	CAPLUS
Brumfitt, W	1994		215	Drugs Exp Clin Res	CAPLUS
Cava, M	1985	41	5061	Tetrahedron	CAPLUS
Dresser, L	1998	18	456	Pharmacotherapy	CAPLUS
Gregory, W	1989	32	1673	J Med Chem	CAPLUS
Gregory, W	1990	33	2569	J Med Chem	CAPLUS
Hiramatsu, K	1997	40	135	J Antimicrob Chemoth	CAPLUS
Lin, A	1997	41	2127	Antimicrob Agents Ch	CAPLUS
National Committee For	2000	20		Approved Standard, 5	
Schmidhammer, H	1982	60	3055	Can J Chem	CAPLUS
Seneci, P	1994		2345	J Chem Soc, Perkin T	CAPLUS
Service, R	1995	270	724	Science	CAPLUS
Shinabarger, D	1997	41	2132	Antimicrob Agents Ch	CAPLUS
Spera, R	1994	48	678	Drugs	
Stinson, S	1996		75	Chem Eng News	
Swaney, S	1998	42	3251	Antimicrob Agents Ch	CAPLUS
Swartz, M	1994	91	2420	Proc Natl Acad Sci U	MEDLINE
Tokuyama, R	2001	49	347	Chem Pharm Bull	CAPLUS
Tokuyama, R	2001	49	353	Chem Pharm Bull	CAPLUS
Tokuyama, R	2001	49	361	Chem Pharm Bull	CAPLUS
Tomasz, A	1994	330	1247	N Engl J Med	MEDLINE
Vaultier, A	1983	24	763	Tetrahedron Lett	
Waldvogel, F	1999	340	556	N Engl J Med	MEDLINE

L41 ANSWER 7 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 130:167984 CASREACT
TI Formation of a **Macrobicyclic** Tris(disulfide) by Molecular Self-Assembly
AU Tam-Chang, Suk-Wah; Stehouwer, Jeffrey S.; Hao, Jinsong
CS Department of Chemistry, University of Nevada, Reno, NV, 89557, USA
SO Journal of Organic Chemistry (1999), 64(2), 334-335
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal

LA English

AB By appropriate mol. design it is possible to enhance the stability of a dimeric tris(disulfide) carcerand which we have observed in equilibrium with the oligomer. The result is a macrobicyclic capsule having a cavity size large enough to accommodate small guest mols.

RX(3) OF 21 ...**F** ===> I...



F

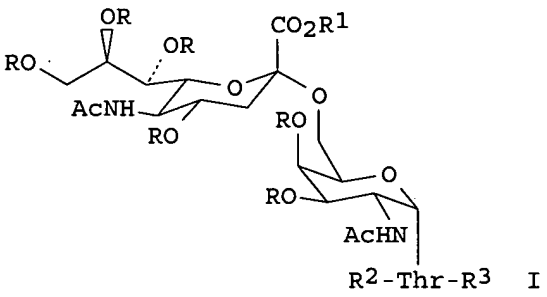
I
YIELD 100%

RX(3) RCT F **190779-62-5**
RGT J 14044-65-6 BH3-THF
PRO I 149525-65-5

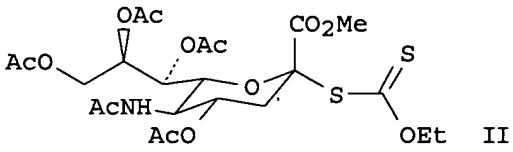
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Anon				no publication given	
Anon				no publication given	
Anon				no publication given	
Anon				no publication given	
Bisson, A	1997	36	2340	Angew Chem, Int Ed E	CAPLUS
Burns, J	1990	112	6296	J Am Chem Soc	CAPLUS
Conn, M	1997	97	1647	Chem Rev	CAPLUS
Gilbert, H	1995	252	8	Methods Enzymol	
Houk, J	1987	109	6825	J Am Chem Soc	CAPLUS
Houk, J	1987	143	129	Methods Enzymol	CAPLUS
Houk, J	1989	45	91	Tetrahedron Lett	CAPLUS
Lawrence, D	1995	95	2229	Chem Rev	CAPLUS
Lees, W	1993	58	642	J Org Chem	CAPLUS
Lehn, J	1994	66	1961	Pure Appl Chem	CAPLUS
Lindsey, J	1991	15	153	New J Chem	CAPLUS
Metzger, A	1997	36	862	Angew Chem, Int Ed E	CAPLUS
Pappas, J	1979		67	J Chem Soc, Perkin T	CAPLUS
Philp, D	1996	35	1154	Angew Chem, Int Ed E	
Rosenfield, R	1977	99	4860	J Am Chem Soc	CAPLUS
Rowan, S	1997	119	2578	J Am Chem Soc	CAPLUS
Singh, R	1990	112	1190	J Am Chem Soc	CAPLUS
Stack, T	1993	115	6466	J Am Chem Soc	CAPLUS
Stang, P	1997	30	502	Acc Chem Res	CAPLUS
Tecilla, P	1995	51	435	Tetrahedron	CAPLUS
Timmerman, P	1997	3	1823	Chem Eur J	CAPLUS
Vogtle, F	1974	13	814	Angew Chem, Int Ed E	
Whitesides, G	1995	28	37	Acc Chem Res	CAPLUS
Yang, J	1993	115	5314	J Am Chem Soc	CAPLUS
Ziegler, D	1985	54	305	Annu Rev Biochem	MEDLINE

L41 ANSWER 8 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 126:343855 CASREACT
TI Solid-phase synthesis of a tumor-associated **sialyl-TN** antigen glycopeptide with a partial sequence of the "tandem repeat" of the MUC-1 mucin
AU Liebe, Beate; Kunz, Horst
CS Inst. Org. Chem. Univ., Mainz, D-55128, Germany
SO Angewandte Chemie, International Edition in English (1997), 36(6), 618-621
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI



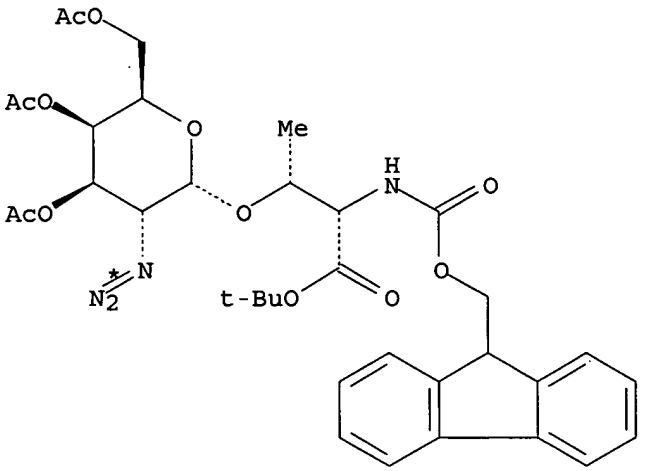
I



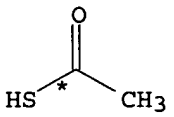
II

AB The solid-phase preparation of undecapeptide I (R = R1 = H, R2 = Ac-Ala-Pro-Pro-Ala-His-Gly-Val; R3 = Ser-Ala-Pro-OH) was achieved in 42% overall yield using a HYCRAM allylic linker on an (aminomethyl)polystyrene resin and 9-fluorenylmethoxycarbonyl (Fmoc) chemical Fmoc-sialyl-TN-threonine building block I (R = Ac, R1 = Me, R2 = Fmoc, R3 = OH) was prepared in 5 steps from Fmoc-Thr-OCMe3, 3,4,6-tri-O-acetyl-2-azido-2-deoxy-α-D-galactopyranosyl bromide, and sialyl-xanthogenate II.

RX(1) OF 15 ...**A** + **B** ===> **C**...



A



B

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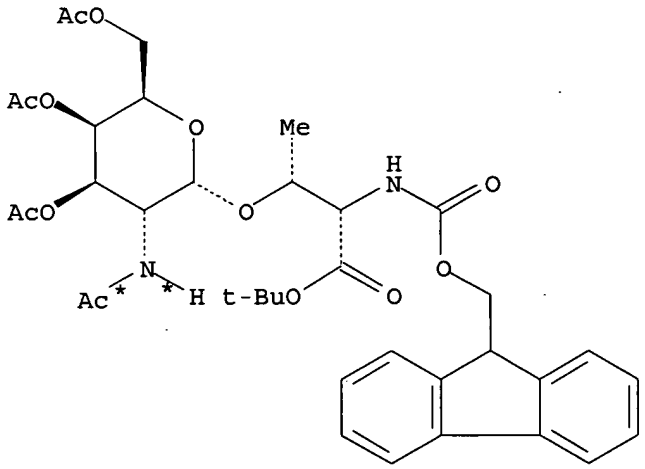


C

RX(1) RCT A **120791-77-7**, B **507-09-5**
PRO C **120173-56-0**

RETABLE

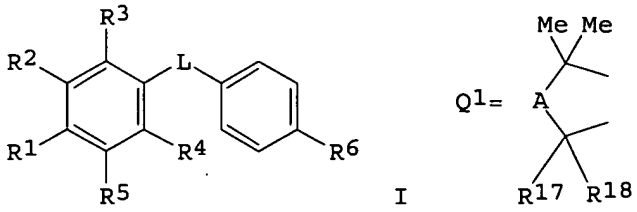
Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Birberg, W	1991	32	7457	Tetrahedron Lett	CAPLUS
Braum, G	1991			Ph D dissertation, U	
Dasgupta, F	1988	177	c13	Carbohydr Res	CAPLUS
Dippold, W	1990			Ph D dissertation, U	
Elofsson, M	1995	36	7499	Tetrahedron Lett	CAPLUS
Gendler, S	1990	265	15286	J Biol Chem	CAPLUS
Gold, D	1988	9	137	Tumor Biol	MEDLINE
Hakomori, S	1991	43	646	Curr Opin Immunol	
Hanisch, F	1989	264	872	J Biol Chem	CAPLUS
Iijima, H	1988	172	183	Carbohydr Res	CAPLUS
Knorr, R	1989	30	1927	Tetrahedron Lett	CAPLUS

Kunz, H	1984	96	49	Angew Chem	CAPLUS
Kunz, H	1986	98	354	Angew Chem	CAPLUS
Kunz, H	1984	23	71	Angew Chem Int Ed En	
Kunz, H	1986	25	360	Angew Chem Int Ed En	
Kunz, H	1990	202	207	Carbohydr Res	CAPLUS
Kurosaka, A	1988	263	8724	J Biol Chem	CAPLUS
Liebe, B	1994	35	8777	Tetrahedron Lett	CAPLUS
Marra, A	1989	187	35	Carbohydr Res	CAPLUS
McLean, G	1994	4	249	Can J Oncol	
Nakahara, Y	1991	216	211	Carbohydr Res	CAPLUS
Paulsen, H	1982	109	89	Carbohydr Res	CAPLUS
Schultz, M	1993	4	1205	Tetrahedron:Asymmetr	CAPLUS
Seitz, O	1995	107	901	Angew Chem	
Seitz, O	1995	34	803	Angew Chem Int Ed En	CAPLUS
Stadie, T	1995	229	140	Eur J Biochem	CAPLUS
Toyokuni, T	1995	24	231	Chem Soc Rev	CAPLUS

L41 ANSWER 9 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 114:42807 CASREACT
TI Preparation of **diarylheterocycles** as drugs and cosmetics
IN Wuest, Hans Heiner; Janssen, Bernd
PA BASF A.-G., Germany
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3903993	A1	19900816	DE 1989-3903993	19890210
	EP 382077	A2	19900816	EP 1990-101947	19900201
	EP 382077	A3	19910731		
	EP 382077	B1	19950517		
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
	CA 2009604	AA	19900810	CA 1990-2009604	19900208
	CA 2009604	C	20010102		
	US 5061705	A	19911029	US 1990-476875	19900208
	JP 02240058	A2	19900925	JP 1990-28617	19900209
	JP 2930645	B2	19990803		
	US 5196532	A	19930323	US 1991-717264	19910618
	US 5206242	A	19930427	US 1991-753916	19910903
	US 5338749	A	19940816	US 1992-972518	19921106
	US 5475017	A	19951212	US 1994-242415	19940513
PRAI	DE 1989-3903993	19890210			
	US 1990-476875	19900208			
	US 1991-717264	19910618			
	US 1992-972518	19921106			

OS MARPAT 114:42807
GI



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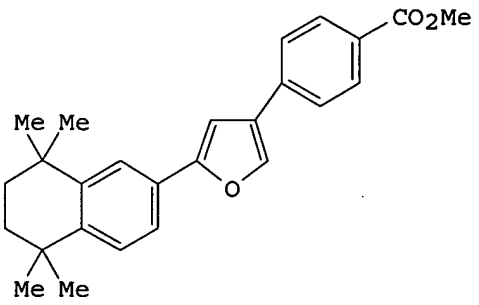
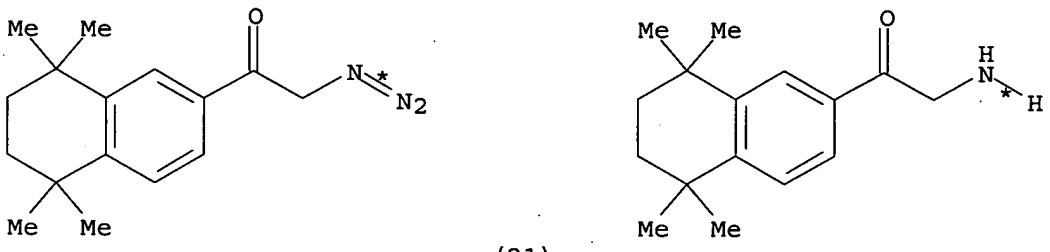


II

AB The title compds. [I; R1 = H, OH, R2 = Me3C; R1R2 = Q1; A = (Me-, HO-, or O-substituted) CH2, CH2CH2; L = (HO-, HS-, alkyl-, or alkanoyl-substituted) heterocyclyl; R3 = H, OH, alkoxy; R4 = H, alkyl, halo, MeO; R5 = H, MeO, Me3C; R6 = H, Me, cyano, alkylthio, alkylsulfinyl, alkylsulfonyl, hydroxymethyl, etc.; R17, R18 = H, Me] were prepared as drugs and cosmetics (no data). Thus, 6-acetyl-1,2,3,4-tetrahydro-1,1,4,4-tetramethylnaphthalene and 4-HCOC6H4CO2Me were stirred 16 h in **MeOH** containing NaOH to give 3-(4-carbomethoxyphenyl)-1-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-propen-1-one. The latter was stirred with MeNO2 and Triton B in **MeOH** to give a residue which in CH2Cl2/THF at -25° was treated with NaOMe in **MeOH** . The resulting solution was added to a -25° solution of H2SO4 in **MeOH** to give 3-(4-carbomethoxyphenyl)-4-dimethoxy-1-(5,5,8,8-tetramethyl-2-naphthalenyl)-1-butanone. The latter was stirred 12 h in concentrated H2SO4 at 25° to give furan-containing title compound II. I are claimed to be useful against skin disorders, precancerous lesions, tumors, rheumatic and arthritic disease, dry eye, etc.

RX(21) OF 35 ...**BB** ===> BE



BB

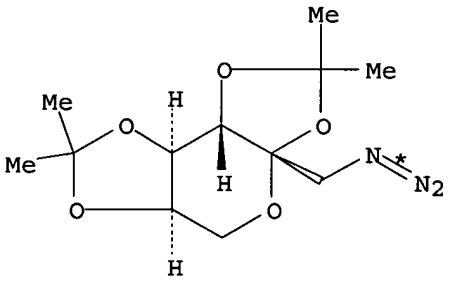
BE

RX(21) RCT BB **131331-90-3**

RGT BF 7647-01-0 HCl
PRO BE 131331-91-4
SOL **67-56-1** MeOH

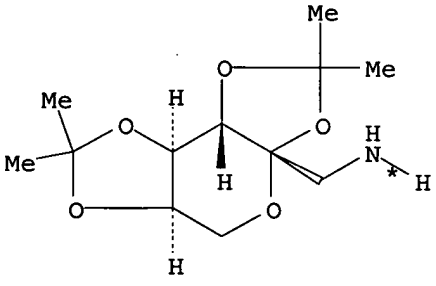
L41 ANSWER 10 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 113:59693 CASREACT
TI Preparation of 1-(**azidoaryl**)amido- and 1-(**azidoaryl**)thio-1-deoxy-D-fructose analogs
AU Goodwin, James C.
CS North. Reg. Res. Cent., Agric. Res. Serv., Peoria, IL, 61604, USA
SO Carbohydrate Research (1989), 195(1), 150-6
CODEN: CRBRAT; ISSN: 0008-6215
DT Journal
LA English
AB Extension of photoaffinity labeling to D-fructose resulted in the syntheses of 1-(4-azido-2-hydroxybenzamido)-1-deoxy-β-D-fructose and 1-(4-azido-2-nitrophenyl)thio-1-deoxy-β-D-fructose as potential photoprobes to study the mechanism for transport of D-fractose in corn endosperm.

RX(1) OF 12 **A** ===> B...



A

(1) ⟶



B
YIELD 91%

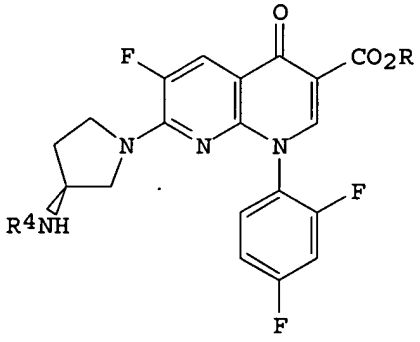
RX(1) RCT A **78574-36-4**
RGT C 1333-74-0 H2
PRO B 128316-82-5
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH

L41 ANSWER 11 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

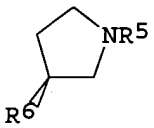
AN 112:139018 CASREACT
TI Process for the preparation of enantiomerically pure (aminopyrrolidinyl) **naphthyridine**- and -quinolonecarboxylic acids as bactericides
IN Chu, Daniel Tim Wo; Rosen, Terry Jay
PA Abbott Laboratories, USA
SO Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 331960	A2	19890913	EP 1989-102927	19890220
	EP 331960	A3	19910123		
	EP 331960	B1	19940518		
	R: BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
	US 4859776	A	19890822	US 1988-167058	19880311
	ES 2056130	T3	19941001	ES 1989-102927	19890220
	JP 01316349	A2	19891221	JP 1989-57657	19890309
	CA 1338892	A1	19970204	CA 1989-593374	19890310
	US 4956475	A	19900911	US 1989-356970	19890525
	US 5099032	A	19920324	US 1990-531816	19900601
	US 5359088	A	19941025	US 1993-39545	19930329
PRAI	US 1988-167058	19880311			
	US 1989-356970	19890525			
	US 1990-531816	19900601			
	US 1992-844262	19920302			

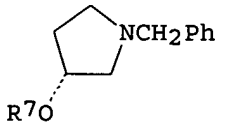
OS MARPAT 112:139018
GI



I



III

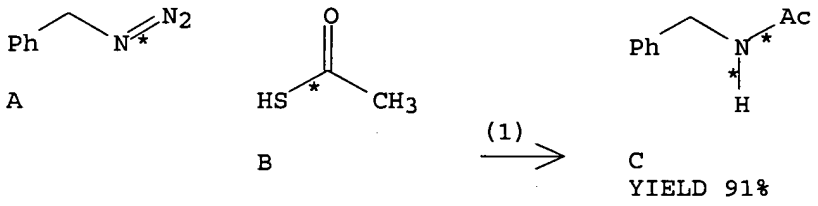


V

AB The title compds., specifically (I; R = R4 = H) (II), having antibacterial activity, are prepared by reaction of an enantiomerically pure N-1 protected (S)-3-aminopyrrolidine (III; R5 = H; R6 = protected NH2) with 7-chloro-1-(o,p-difluorphenyl)-1,4-dihydro-6-fluoro-4-oxo-1,8-naphthyridine-3-carboxylic acid (IV) or its ester. Thus, mesylation of (R)-3-hydroxypyrrolidine derivative (V; R7 = H) with MeSO2cl in CH2Cl2 containing Et3N gave V (R6 = MeSO2) which was heated 3 h at 65° with Bu4NN3 in MeCN to give III (R5 = CH2Ph, R6 = N3). Reductive acetylation of the

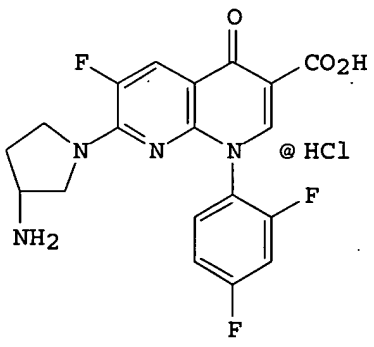
latter with thiolacetic acid at room temperature for 5 h gave III (R5 = CH2Ph, R6 = NHAc) which was hydrogenolyzed over 20% Pd/C in **MeOH** to give III (R5 = H, R6 = AcNH). This was heated 21 h at 65° with Et ester of IV in pyridine containing Et3N to give I (R = Et, R4 = Ac) which was saponified 2 h at 65° with 1M aqueous NaOH-THF and then refluxed in 6M HCl to give II.HCl. This in mice showed ED50 of 0.2, 8.6, and 0.4 mg/kg/day s.c. against Escherichia coli Juhl, Pseudomonas aeruginosa 5007, and Staphylococcus aureus NCTC 10649, resp., while a racemic mixture of II.HCl showed ED50 of 0.3, >20, and 0.4 mg/kg/day against the same bacteria, resp. Reductive acetylation of various azide compds. with thiolacetic acid to acetamides were also described.

RX(1) OF 16 **A** + **B** ===> **C**

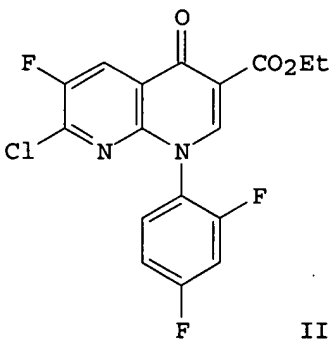


RX(1) RCT A **622-79-7**, B **507-09-5**
PRO C **588-46-5**

L41 ANSWER 12 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 109:54686 CASREACT
TI **Asymmetric** synthesis and properties of the enantiomers of the antibacterial agent 7-(3-aminopyrrolidin-1-yl)-1-(2,4-difluorophenyl)-1,4-dihydro-6-fluoro-4-oxo-1,8-**naphthyridine**-3-carboxylic acid hydrochloride
AU Rosen, Terry; Chu, Daniel T. W.; Lico, Isabella M.; Fernandes, Prabhavathi B.; Shen, Linus; Borodkin, Saul; Pernet, Andre G.
CS Abbot Lab., Abbott Park, IL, 60064, USA
SO Journal of Medicinal Chemistry (1988), 31(8), 1586-90
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I

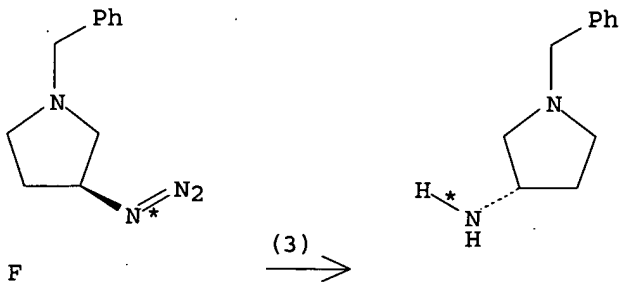


II

AB The title compound (I), a potent member of the quinolonecarboxylic acid class of antibacterial agents, was prepared as its enantiomers from N-benzylpyrroline and naphthyridine II. (S)-(+)-I is 1-2 log2 dilns. more

active than (R)-(-)-I against aerobic bacteria and 1-2 or more log2 dilns. more active against anaerobic bacteria in vitro. (S)-(+)-I shows significantly better in vivo activity in a Pseudomonas aeruginosa mouse protection model compared to (±)-I. Coupled with the improved solubility profile of (S)-(+)-I relative to racemic material, these features may be of practical significance from a clin. standpoint.

RX(3) OF 61 ...**F** ===> I...

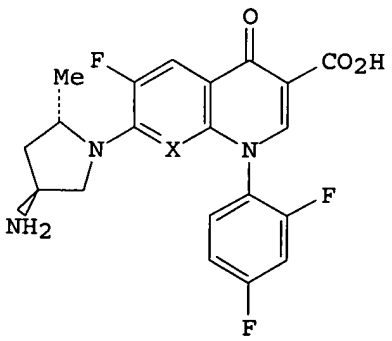


F

I
YIELD 93%

RX(3) RCT F **114636-29-2**
RGT J 1333-74-0 H2
PRO I 114715-38-7
CAT 7440-06-4 Pt
SOL **67-56-1** MeOH

L41 ANSWER 13 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 109:54632 CASREACT
TI **Design**, synthesis, and properties of (4S)-7-(4-amino-2-substituted-pyrrolidin-1-yl)quinolone-3-carboxylic acids
AU Rosen, Terry; Chu, Daniel T. W.; Lico, Isabella M.; Fernandes, Prabhavathi B.; Marsh, Kennan; Shen, Linus; Cepa, Valerie G.; Pernet, Andre G.
CS Med. Chem. Dep., Pfizer, Groton, CT, 06340, USA
SO Journal of Medicinal Chemistry (1988), 31(8), 1598-611
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI

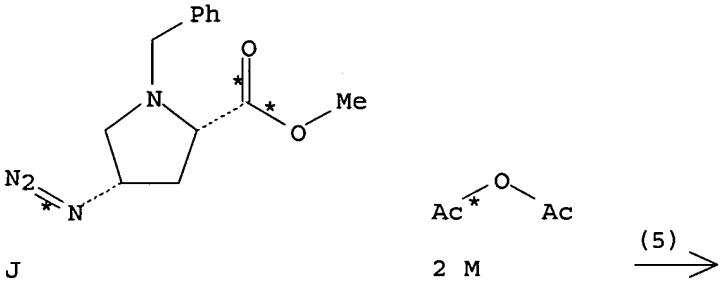


I

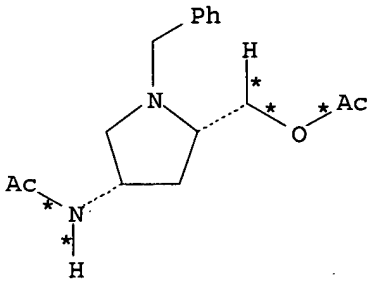
AB A series of enantiomerically homogeneous title compds. e.g. I (X = CH) were prepared, in an effort to utilize the 2-position of the pyrrolidine

moiety to improve upon the solubility and pharmacokinetic properties while still maintaining potent antibacterial activity. The absolute stereochem. at the 2-position of the pyrrolidine ring is critical to the maintenance of such activity. Full details of the asym. synthesis and the in vitro and in vivo structure-activity relationships of this series of compds. are reported as well as the physicochem. properties, such as water solubility and log P, associated with the structural modifications. Pharmacokinetic properties of several of these compds. in mice and the pharmacokinetics of I, which has the best overall properties of agents in this study, in dogs are discussed.

RX(5) OF 348 ...**J** + 2 M ===> **N**...



J 2 M



N

RX(5) RCT J **113451-53-9**

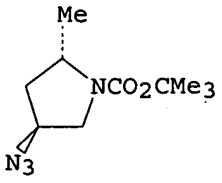
STAGE(1)
RGT O 16853-85-3 LiAlH4
SOL 109-99-9 THF

STAGE(2)
RCT M 108-24-7
RGT D 121-44-8 Et3N

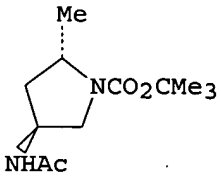
PRO N **114676-50-5**

L41 ANSWER 14 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 108:150212 CASREACT
TI A convenient and highly **chemoselective** method for the reductive acetylation of azides
AU Rosen, Terry; Lico, Isabella M.; Chu, Daniel T. W.
CS Anti-Infect. Res. Div., Abbott Lab., Abbott Park, IL, 60064, USA
SO Journal of Organic Chemistry (1988), 53(7), 1580-2
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal

LA English
GI



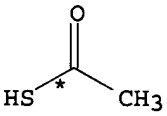
I



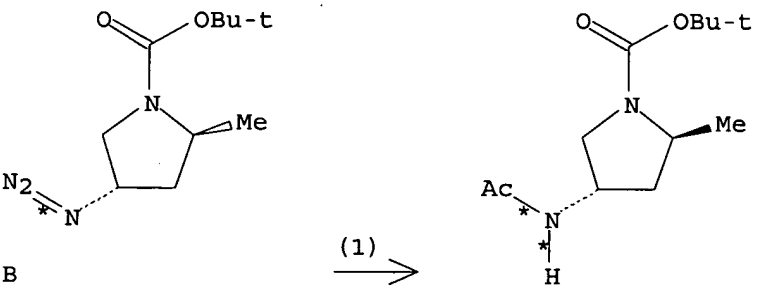
II

AB Azides, e.g. I, react with AcSH to afford the corresponding acetamides, e.g. II, in good yield. The reaction is highly chemoselective. The transformation occurs under extremely mild conditions and has been accomplished in the presence of a wide variety of functional groups including tert-butoxycarbonyl and benzyl protecting groups, olefins, carboxylic esters and a methanesulfonate ester. This rapid reductive acetylation allows the introduction of a protected amino group into a mol. possessing functionality otherwise incompatible with the free amine.

RX(1) OF 9 **A** + **B** ===> **C**



A



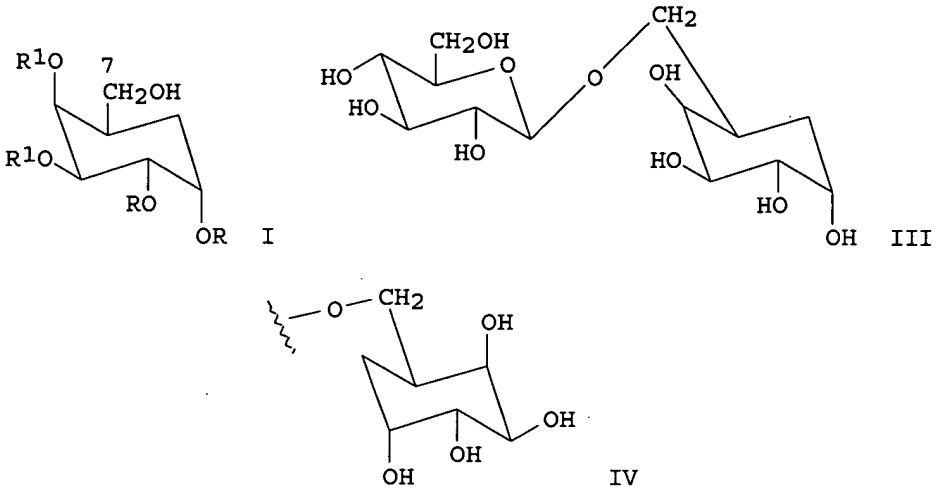
B

C
YIELD 84%

RX(1) RCT A **507-09-5**, B **113451-51-7**
PRO C **113451-55-1**

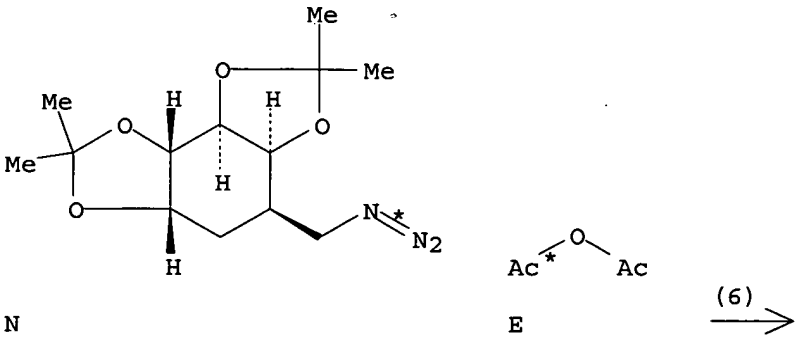
L41 ANSWER 15 OF 15 CASREACT COPYRIGHT 2005 ACS on STN
AN 108:56453 CASREACT
TI **Pseudo-sugars.** Part XVIII. Synthesis of some derivatives of pseudo-α-galactopyranose [(1,2/3,4,5)-5-(hydroxymethyl)-1,2,3,4-cyclohexanetetrol]
AU Ogawa, Seiichiro; Shibata, Yasushi; Miyazawa, Keiko; Toyokuni, Tatsushi;

Iida, Tatsuo; Sumai, Tetsuo
CS Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan
SO Carbohydrate Research (1987), 163(1), 53-62
CODEN: CRBRAT; ISSN: 0008-6215
DT Journal
LA English
GI

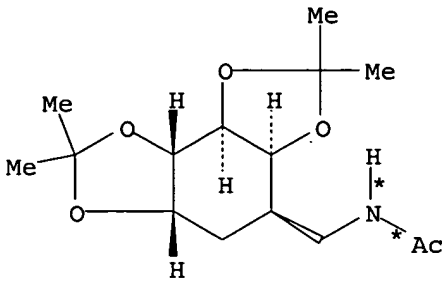


AB Isopropylidenation of DL-(1,2/3,4,5)-5-hydroxymethyl-1,2,3,4-cyclohexanetetrol (I; R = R1 = H) with Me2C(OMe)2 in DMF in the presence of p-toluenesulfonic acid gave the 1,2:3,4-, 1,2;4,7-, and 2,3:4,7-di-O-isopropylidene derivs. Several C-7 substituted derivs. of I (R = R1 = H) of biol. interest were prepared by nucleophilic displacement reactions of the tosylate derived from the most readily available 1,2:3,4-di-O-isopropylidene derivative (I; R2 = R12 = Me2C) (II). Condensation of II with 2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl bromide gave diastereoisomeric products, which were converted into 7-O-(β-D-glucopyranosyl)-pseudo-α-D-(III) and -L-galactopyranose (IV), the structures of which were confirmed by degradation of the octaacetate of III, yielding the known pseudo-α-D-galactopyranose pentaacetate.

RX(6) OF 83 ...**N** + **E** ===> **P**...



N E (6) →



P
YIELD 73%

RX(6) RCT N **112314-07-5**

STAGE(1)
RGT Q 1333-74-0 H2
CAT 7440-02-0 Ni
SOL 141-78-6 AcOEt

STAGE(2)
RCT E 108-24-7
SOL **67-56-1** MeOH
PRO P **112314-08-6**

=>

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FILE CONTENT:1840 - 1 May 2005 VOL 142 ISS 18

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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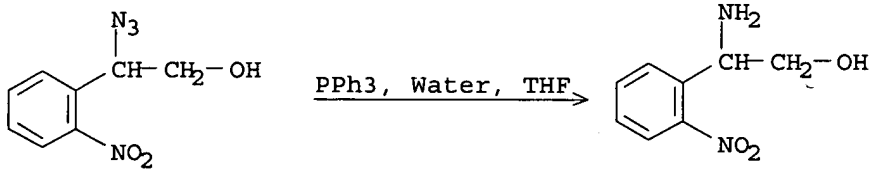
L41 ANSWER 1 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 58



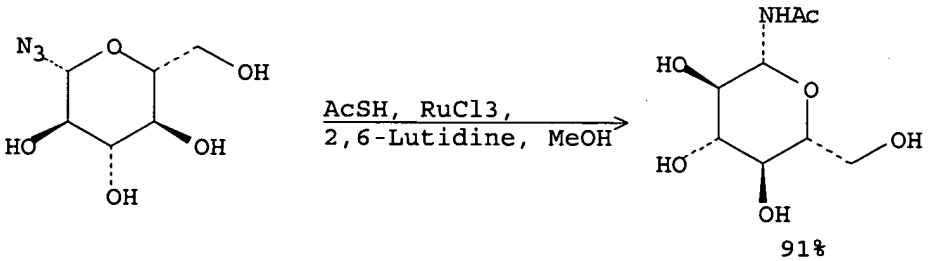
91%

This is a "free" view of "hits" in rep 1-15, L41, Casreact

REF: Bioorganic & Medicinal Chemistry, 12(10), 2749-2757; 2004

L41 ANSWER 2 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 7

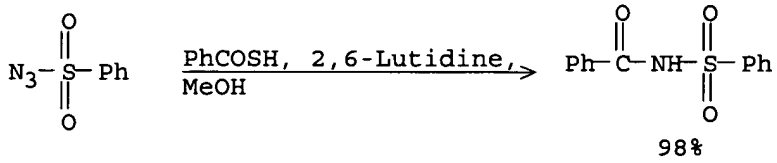


91%

REF: Tetrahedron Letters, 44(51), 9083-9085; 2003
NOTE: yield depends on amt. of cat.

L41 ANSWER 3 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

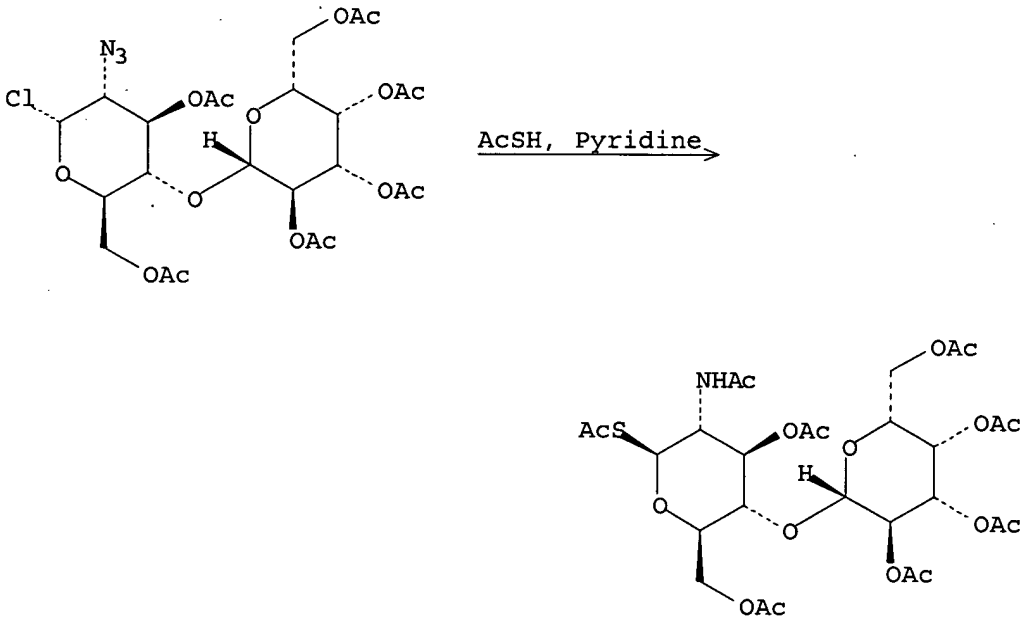
RX(1) OF 30



REF: Journal of the American Chemical Society, 125(26), 7754-7755; 2003

L41 ANSWER 4 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

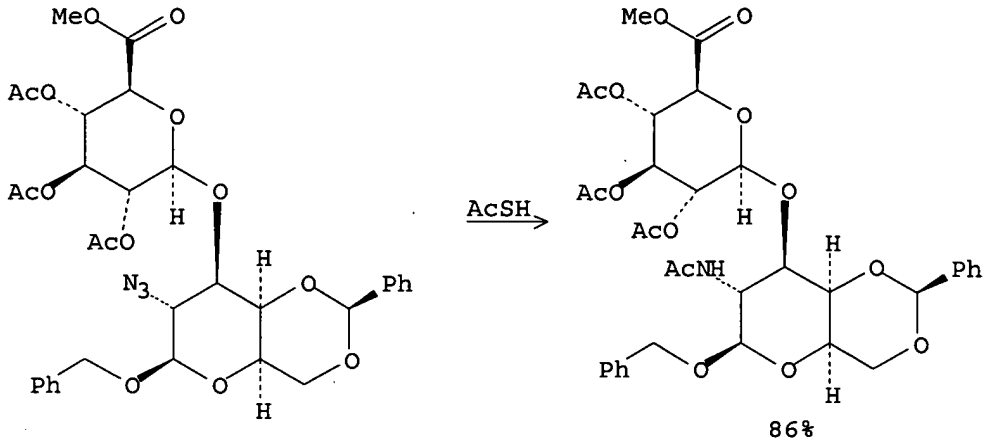
RX(1) OF 20



REF: Tetrahedron Letters, 44(18), 3617-3620; 2003

L41 ANSWER 5 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 59



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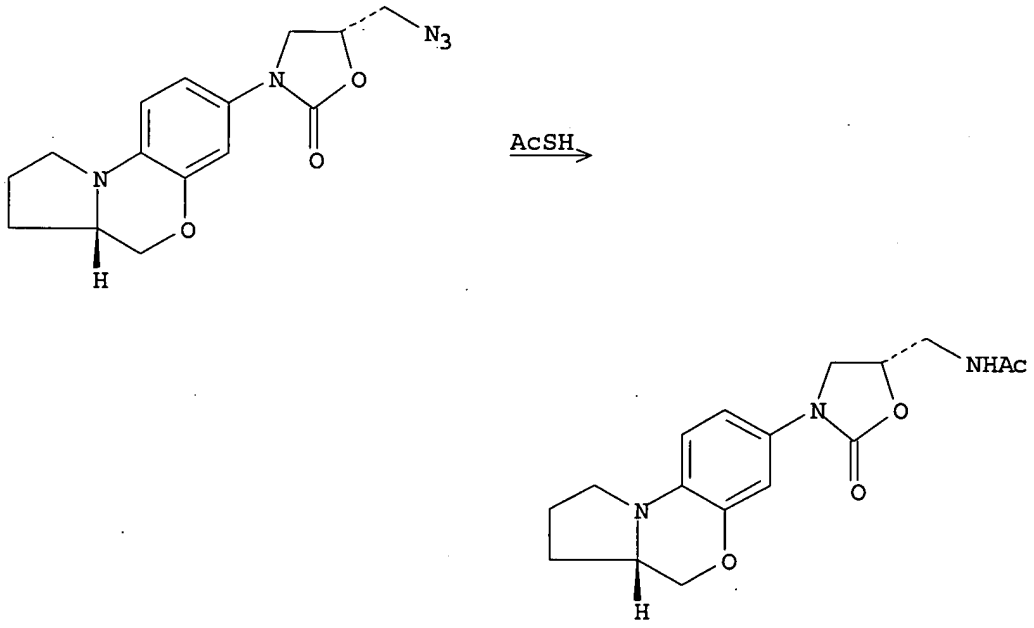
REF: PCT Int. Appl., 2003070960, 28 Aug 2003

L41 ANSWER 6 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 402



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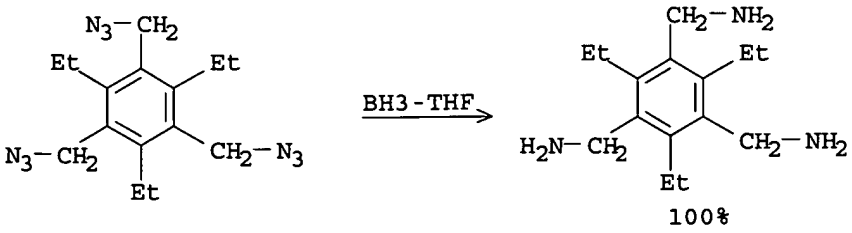
REF: Journal of Medicinal Chemistry, 45(18), 3953-3962; 2002

L41 ANSWER 7 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 21



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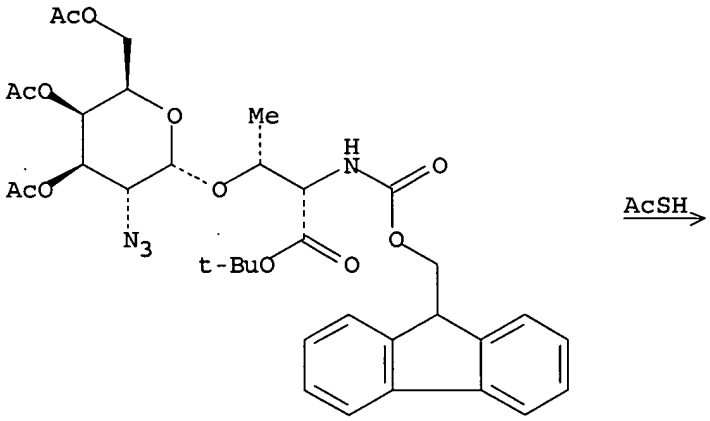
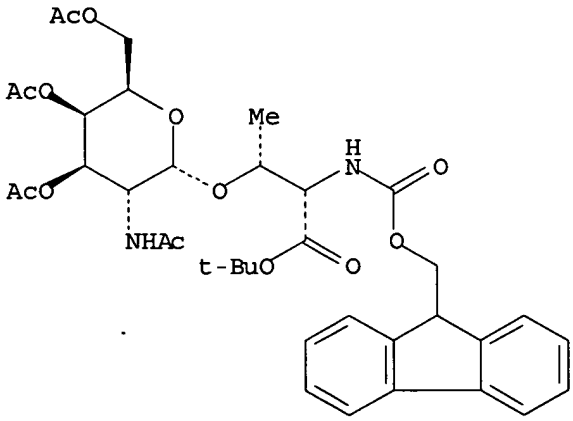
REF: Journal of Organic Chemistry, 64(2), 334-335; 1999

L41 ANSWER 8 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 15



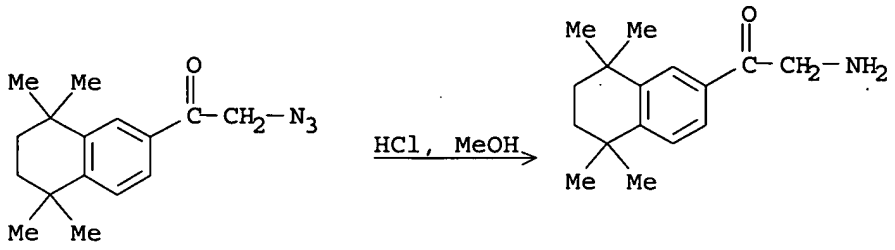
RX(1) OF 15



REF: Angewandte Chemie, International Edition in English, 36(6), 618-621; 1997

L41 ANSWER 9 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

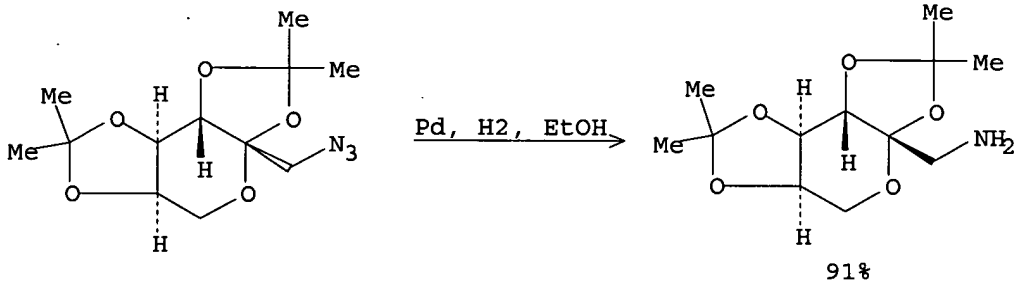
RX(21) OF 35



REF: Ger. Offen., 3903993, 16 Aug 1990

L41 ANSWER 10 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

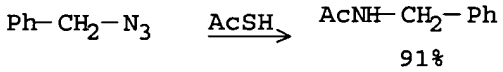
RX(1) OF 12



REF: Carbohydrate Research, 195(1), 150-6; 1989

L41 ANSWER 11 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

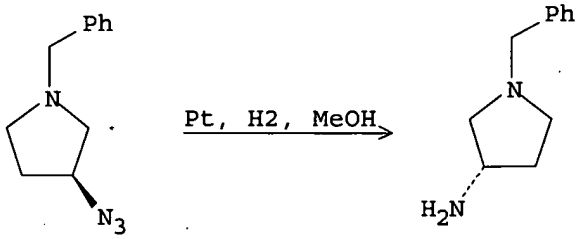
RX(1) OF 16



REF: Eur. Pat. Appl., 331960, 13 Sep 1989

L41 ANSWER 12 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 61



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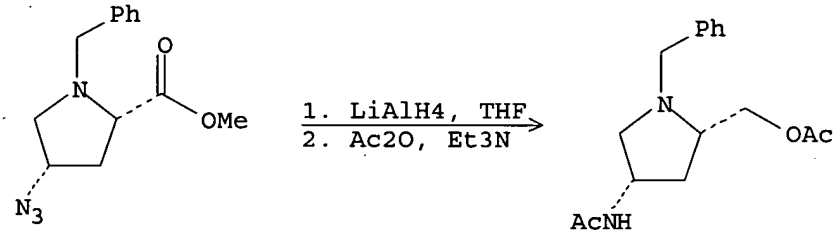
REF: Journal of Medicinal Chemistry, 31(8), 1586-90; 1988

L41 ANSWER 13 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(5) OF 348



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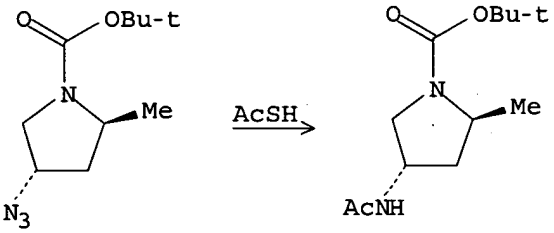
REF: Journal of Medicinal Chemistry, 31(8), 1598-611; 1988

L41 ANSWER 14 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 9



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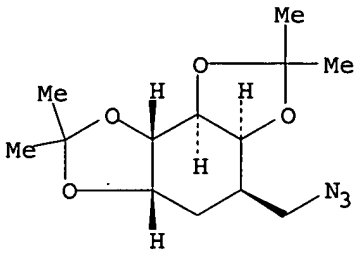
REF: Journal of Organic Chemistry, 53(7), 1580-2; 1988

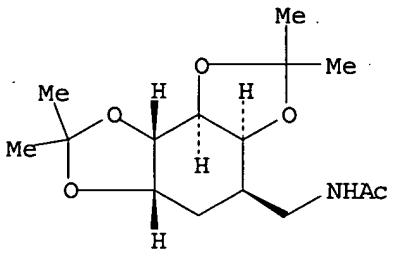
L41 ANSWER 15 OF 15 CASREACT COPYRIGHT 2005 ACS on STN

RX(6) OF 83



1. Ni, H2, AcOEt
2. Ac2O, MeOH

(step 1)



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REF: Carbohydrate Research, 163(1), 53-62; 1987

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=> d all hitstr tot

L63 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:425546 HCAPLUS
DN 141:53768
ED Entered STN: 27 May 2004
TI New reaction for peptide bond formation by merely mixing. New amidation by condensation of thiocarboxylic acid and azide compounds

AU Chino, Masao
CS Mitsubishi Well Pharma Co., Ltd., Japan
SO Kagaku to Kogyo (Tokyo, Japan) (2004), 57(5), 531
CODEN: KAKTAF; ISSN: 0022-7684
PB Nippon Kagakkai
DT Journal; General Review
LA Japanese
CC 21-0 (General Organic Chemistry)
AB A review on preparation of amides by mixing thiocarboxylic acid with azides in the presence of 2,6-lutidine.
ST review amidation thiocarboxylic acid azide; peptide bond formation thiocarboxylic acid azide review
IT Amidation
(amidation by mixing thiocarboxylic acids with azides)
IT **Azides**
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by mixing thiocarboxylic acids with azides)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(amidation by mixing thiocarboxylic acids with azides)
IT **Carboxylic acids, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**thiocarboxylic**; amidation by mixing **thiocarboxylic** acids with azides)

L63 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:899646 HCAPLUS
DN 140:128580
ED Entered STN: 18 Nov 2003
TI RuCl3-promoted amide formation from azides and **thio-acids**
AU Fazio, Fabio; Wong, Chi-Huey
CS Department of Chemistry and Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Tetrahedron Letters (2003), 44(51), 9083-9085
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science B.V.
DT Journal
LA English
CC 33-7 (Carbohydrates)
Section cross-reference(s): 21, 67
OS CASREACT 140:128580
AB Described here is the Ru(III)-promoted amide formation from sugar azides and **thio-acids**, (e.g., thiolacetic acid) which were shown not to form amides at room temperature in the absence of ruthenium. We believe that a complex formed by Ru(III) increases the reactivity of the thiocarbonyl species and therefore reaction with azides occurs at room temperature, even when less reactive (electron rich and/or sterically hindered) azides are employed.
ST sugar azide thiolacetic acid ruthenium trichloride prepn carbohydrate amide; reaction mechanism ruthenium catalyst azide thioacid prepn amide
IT Catalysts
Reaction mechanism
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT **Azides**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT Carbohydrates, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as

promoter)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT **Carboxylic acids, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**thiocarboxylic**; preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT 10049-08-8, Ruthenium trichloride
RL: CAT (Catalyst use); USES (Uses)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT **507-09-5**, Thiolacetic acid, reactions 6205-69-2 13992-25-1
20379-59-3, β-D-Glucopyranosyl azide 29847-23-2 140428-81-5
165331-08-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
IT 6205-71-6P 6205-72-7P 6983-35-3P 6983-36-4P 173143-13-0P
648887-44-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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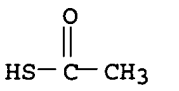
IT **507-09-5**, Thiolacetic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from sugar azides and thiolacetic acid using RuCl3 as promoter)
RN 507-09-5 HCAPLUS
CN Ethanethioic acid (9CI) (CA INDEX NAME)



L63 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:505304 HCAPLUS
DN 139:213881
ED Entered STN: 03 Jul 2003
TI The Reaction of **Thio Acids** with Azides: A New Mechanism and New Synthetic Applications
AU Shangguan, Ning; Katukojvala, Sreenivas; Greenberg, Rachel; **Williams, Lawrence J.**
CS Department of Chemistry and Chemical Biology, Rutgers The State University of New Jersey, Piscataway, NJ, 08854, USA
SO Journal of the American Chemical Society (2003), 125(26), 7754-7755
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society

DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 139:213881
AB A new amide synthesis strategy based on a fundamental mechanistic revision of the reaction of **thio acids** and organic azides is presented. It was shown that amines are not formed as intermediates in this reaction, and alternative mechanisms proceeding through a thiatriazoline intermediate are suggested. The reaction has been applied to the preparation of both simple and architecturally complex amides that are difficult to access using conventional methods. The reaction is chemoselective, effective for unprotected substrates, and compatible with aprotic and protic solvents, including water.
ST amide prepn; sulfonamide acyl prepn; acid thio coupling azide
IT Sulfonamides
RL: SPN (Synthetic preparation); PREP (Preparation)
(acyl; preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT **Azides**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT **Carboxylic acids, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**thiocarboxylic**; preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT **98-91-9**, **Thiobenzoic acid 507-09-5**, **Thioacetic acid**, reactions 622-79-7, Benzyl azide 938-10-3, Phenylsulfonyl azide **941-55-9**, Tosyl azide 3422-03-5 16722-99-9, β-Azido styrene 17202-49-2 20379-59-3, β-D-Glucopyranosyl azide 28166-06-5, 4-Fluoro-3-nitrophenyl azide **30516-87-1** 33639-93-9 77422-70-9 106531-68-4, Dansyl azide 263764-96-1 586957-49-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT 351-32-6P 588-46-5P 1485-70-7P 3559-04-4P 5661-14-3P 6983-36-4P 15354-97-9P 15355-08-5P 18793-44-7P 35922-92-0P 38091-74-6P 58379-67-2P 69261-50-3P 70465-85-9P 75893-06-0P 78007-47-3P 103324-91-0P 131098-83-4P 228425-41-0P 329775-56-6P 586957-47-3P 586957-48-4P 586957-50-8P 586957-51-9P 586957-55-3P 586957-56-4P 586957-57-5P 586957-58-6P 586957-59-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
IT 586957-52-0 586957-53-1 586957-54-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(thioester cleavage; preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
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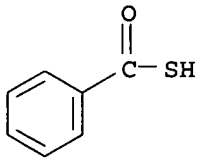
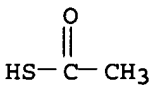
IT **98-91-9**, **Thiobenzoic acid 507-09-5**, **Thioacetic acid**, reactions **941-55-9**, Tosyl azide **30516-87-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides, carbamates and N-acyl and α-aminoacyl sulfonamides via coupling of **thio acids** with azides)

RN 98-91-9 HCAPLUS
CN Benzenecarbothioic acid (9CI) (CA INDEX NAME)

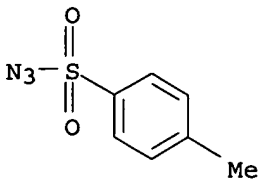


RN 507-09-5 HCAPLUS
CN Ethanethioic acid (9CI) (CA INDEX NAME)



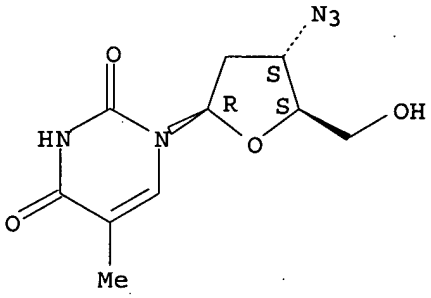
RN 941-55-9 HCAPLUS

CN Benzenesulfonyl azide, 4-methyl- (9CI) (CA INDEX NAME)



RN 30516-87-1 HCAPLUS
CN Thymidine, 3'-azido-3'-deoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L63 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:437855 HCAPLUS
DN 139:323413
ED Entered STN: 09 Jun 2003
TI Esters and amides from activated alcohols using manganese(IV) dioxide: Tandem oxidation processes
AU Foot, Jonathan S.; Kanno, Hisashi; Giblin, Gerard M. P.; Taylor, Richard J. K.
CS Department of Chemistry, University of York, York, YO10 5DD, UK
SO Synthesis (2003), (7), 1055-1064
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 23, 24, 25, 26
OS CASREACT 139:323413
AB Manganese(IV) dioxide can be used in conjunction with sodium cyanide in THF-methanol or in methanol alone for the direct conversion of activated alcs. into Me esters. Et and iso-Pr esters can also be prepared Similarly, use of manganese(IV) dioxide and sodium cyanide in THF containing ammonia or primary amines can be used to convert alcs. into the corresponding amides. Several activated alcs. and one non-activated alc. example are reported. For example, reaction of (2E,4E)-2,4-dodecadien-1-ol in the presence of 2-methyl-1-propanamine gave (2E,4E)-N-(2-methylpropyl)-2,4-dodecadienamide in 51% yield.
ST ester amide prepn oxidn alc manganese dioxide sodium cyanide; amide prepn oxidn alc manganese dioxide sodium cyanide; oxidizing agent manganese dioxide sodium cyanide oxidn alc amine
IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(activated alcs.; preparation of esters and amides from activated alcs.

using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alicyclic; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkenyl; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Alicyclic compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(amines; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aralkyl; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Carboxylic acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(aromatic, esters; preparation of esters and amides from activated alcs. using
manganese dioxide and sodium cyanide via tandem oxidation processes)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(aryl; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclic; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Carboxylic acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(esters, alkynyl; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Oxidation
Oxidation
Oxidizing agents
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Esters, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd.; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(unsatd.; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
IT Carboxylic acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(α,β-unsatd., esters; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem

oxidation processes)

IT 112-30-1, 1-Decanol 544-92-3, Copper cyanide (Cu(CN)) 5188-07-8, Methanethiol sodium salt **26628-22-8**, Sodium azide (NaN3)
RL: RCT (Reactant); RACT (Reactant or reagent)
(failed reaction; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)

IT 1885-38-7P, (2E)-3-Phenyl-2-propenenitrile 14371-10-9P, (2E)-3-Phenyl-2-propenal
RL: BYP (Byproduct); PREP (Preparation)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)

IT 74-89-5, Methanamine, reactions 75-31-0, 2-Propanamine, reactions 75-64-9, 2-Methyl-2-propanamine, reactions 78-81-9, 2-Methyl-1-propanamine 97-99-4, Tetrahydrofuran-2-methanol 98-00-0, 2-Furanmethanol 100-51-6, Benzenemethanol, reactions 100-55-0, 3-Pyridinemethanol 105-13-5, 4-Methoxybenzenemethanol 107-11-9, 2-Propen-1-amine 107-19-7, 2-Propyn-1-ol 108-91-8, Cyclohexanamine, reactions 109-89-7, Diethylamine, reactions 123-75-1, Pyrrolidine, reactions 124-40-3, Dimethylamine, reactions 143-33-9, Sodium cyanide 151-50-8, Potassium cyanide (KCN) 333-20-0, Thiocyanic acid potassium salt 586-95-8, 4-Pyridinemethanol 586-98-1, 2-Pyridinemethanol 590-28-3, Cyanic acid potassium salt 619-73-8, 4-Nitrobenzenemethanol 636-72-6, 2-Thiophenemethanol 764-01-2, 2-Butyn-1-ol 873-75-6, 4-Bromobenzenemethanol 928-94-9, (2Z)-2-Hexen-1-ol 928-95-0, (2E)-2-Hexen-1-ol 1313-13-9, Manganese oxide (MnO2), reactions 1504-58-1, 3-Phenyl-2-propyn-1-ol 2408-36-8, Lithium cyanide (Li(CN)) 4407-36-7, (2E)-3-Phenyl-2-propen-1-ol 4412-91-3, 3-Furanmethanol 4568-71-2, 5-(2-Hydroxyethyl)-4-methyl-3-(phenylmethyl)thiazolium chloride 7664-41-7, Ammonia, reactions 7677-24-9, Trimethylsilyl cyanide 7681-82-5, Sodium iodide (NaI), reactions 7758-19-2, Chlorous acid sodium salt 10442-39-4, Tetrabutylammonium cyanide 18485-38-6, (2E,4E)-2,4-Dodecadien-1-ol **34832-35-4**, Ethanethioic acid sodium salt 71637-34-8, 3-Thiophenemethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)

IT 55-21-0P, Benzamide 64-17-5P, Ethanol, preparation 67-63-0P, 2-Propanol, preparation 93-58-3P, Benzoic acid methyl ester 93-60-7P, 3-Pyridinecarboxylic acid methyl ester 121-98-2P, 4-Methoxybenzoic acid methyl ester 611-13-2P, 2-Furancarboxylic acid methyl ester 611-74-5P, N,N-Dimethylbenzamide 613-93-4P, N-Methylbenzamide 619-42-1P, 4-Bromobenzoic acid methyl ester 619-50-1P, 4-Nitrobenzoic acid methyl ester 925-55-3P, (2Z)-3-Cyano-2-propenoic acid methyl ester 1696-17-9P, N,N-Diethylbenzamide 1754-62-7P, (2E)-3-Phenyl-2-propenoic acid methyl ester 1759-68-8P, N-(Cyclohexyl)benzamide 2459-07-6P, 2-Pyridinecarboxylic acid methyl ester 2459-09-8P, 4-Pyridinecarboxylic acid methyl ester 2585-25-3P, N-(2-Methylpropyl)-4-nitrobenzamide 3389-54-6P, 1-Benzoylpyrrolidine 4192-77-2P, (2E)-3-Phenyl-2-propenoic acid ethyl ester 4891-38-7P, 3-Phenyl-2-propynoic acid methyl ester 5440-69-7P, N-(1-Methylethyl)benzamide 5705-57-7P, Benzamide N-(2-methylpropyl) 5894-65-5P, N-(1,1-Dimethylethyl)benzamide 7464-51-9P, 4-Methoxy-N-(2-methylpropyl)benzamide 10283-95-1P, N-(2-Propenyl)benzamide 13894-63-8P, (2E)-2-Hexenoic acid methyl ester 13894-64-9P, (2Z)-2-Hexenoic acid methyl ester 23326-27-4P, 2-Butynoic acid methyl ester 24738-51-0P, (2E,4E)-N-(2-Methylpropyl)-2,4-Dodecadienamide 26218-50-8P, N,N-Dimethyl-3-phenyl-2-Propynamide 60512-85-8P, (2E)-3-Phenyl-2-propenoic acid 1-methylethyl ester 74210-18-7P, N-(2-Methylpropyl)-3-Furancarboxylic acid 78114-53-1P, N-(2-Methylpropyl)-3-Pyridinecarboxamide 92449-52-0P, (2E)-N-(2-Methylpropyl)-3-phenyl-2-propenamide 192988-94-6P, N-(2-Methylpropyl)-2-Thiophenecarboxamide 192988-97-9P, N-(2-Methylpropyl)-3-Thiophenecarboxamide 479352-34-6P, N-(2-Methylpropyl)-4-Pyridinecarboxamide 479352-35-7P,

Tetrahydro-N-(2-methylpropyl)-2-Furancarboxamide 612846-73-8P, (2E)-N-(2-Methylpropyl)-2-hexenamide 612846-75-0P, (2Z)-N-(2-Methylpropyl)-2-hexenamide 612846-77-2P, N-(2-Methylpropyl)-2-Pyridinecarboxamide
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)

RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD

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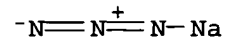
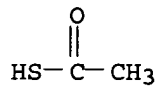
IT **26628-22-8**, Sodium azide (NaN3)
RL: RCT (Reactant); RACT (Reactant or reagent)
(failed reaction; preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
RN 26628-22-8 HCAPLUS
CN Sodium azide (Na(N3)) (9CI) (CA INDEX NAME)



IT **34832-35-4**, Ethanethioic acid sodium salt
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of esters and amides from activated alcs. using manganese dioxide and sodium cyanide via tandem oxidation processes)
RN 34832-35-4 HCAPLUS
CN Ethanethioic acid, sodium salt (9CI) (CA INDEX NAME)



L63 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:640915 HCAPLUS
DN 138:137001
ED Entered STN: 26 Aug 2002
TI A new type of amide formation from thiocarboxylic acid and alkyl azide
AU Park, Sang-Don; Oh, Jung-Hee; Lim, Dongyeol
CS Department of Applied Chemistry, Sejong University, Seoul, 143-747, S. Korea
SO Tetrahedron Letters (2002), 43(36), 6309-6311
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 23
OS CASREACT 138:137001
AB The coupling of thiocarboxylic acid and alkyl azide using various triaryl phosphines was studied. Amide formation greater than 95% was achieved when the free-formation of Staudinger intermediate with electron deficient triaryl phosphines was employed. The coupling of benzenecarbothioic acid with (azidomethyl)benzene in the presence of triphenylphosphine gave N-(phenylmethyl)benzamide in 91% yield. The coupling of (azido)acetic acid Me ester with benzenecarbothioic acid or ethanethioic acid in the presence of arylphosphines gave N-benzoylglycine Me ester and N-acetylglycine Me ester, resp.
ST thiocarboxylic acid azide arylphosphine coupling amide prepn; furanylphosphine thiocarboxylic acid azide coupling amide prepn; phenylphosphine thiocarboxylic acid azide coupling amide prepn; chemoselective coupling thiocarboxylic acid azide arylphosphine amide prepn; benzenecarbothioic acid azide arylphosphine coupling amide prepn; ethanethioic acid azide arylphosphine coupling amide prepn; benzoylglycine prepn benzenecarbothioic acid azidoacetate coupling phenylphosphine;

acetylglycine prepn ethanethioic acid azidoacetate coupling phenylphosphine

IT Phosphines
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl; preparation of amides from thiocarboxylic acid and alkyl azides)

IT Coupling reaction
(chemoselective; preparation of amides from thiocarboxylic acid and alkyl azides)

IT **Azides**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from thiocarboxylic acid and alkyl azides)

IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides from thiocarboxylic acid and alkyl azides)

IT **Carboxylic acids, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**thiocarboxylic**; preparation of amides from **thiocarboxylic** acid and alkyl azides)

IT **98-91-9**, Benzenecarbothioic acid **507-09-5**, Ethanethioic acid, reactions 603-35-0, Triphenylphosphine, reactions 622-79-7, (Azidomethyl)benzene 855-38-9, Tris(4-methoxyphenyl)phosphine 998-40-3, Tributylphosphine 1816-92-8, (Azido)acetic acid methyl ester 5518-52-5, Tri(2-furanyl)phosphine 18437-78-0, Tris(4-fluorophenyl)phosphine 23039-94-3, Tris(3-fluorophenyl)phosphine 56602-33-6, (Benzotriazol-1-yloxy)tris(dimethylamino) hexafluorophosphate 128625-52-5, (1-Hydroxy-1H-benzotriazolato-O)tri-1-pyrrolidinylphosphorus(1+) hexafluorophosphate(1-)
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from thiocarboxylic acid and alkyl azides)

IT 588-46-5P, N-(Phenylmethyl)acetamide 1117-77-7P, N-Acetylglycine methyl ester 1205-08-9P, N-Benzoylglycine methyl ester 1485-70-7P, N-(Phenylmethyl)benzamide
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides from thiocarboxylic acid and alkyl azides)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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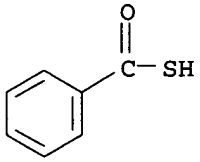
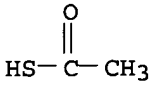
IT **98-91-9**, Benzenecarbothioic acid **507-09-5**, Ethanethioic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amides from thiocarboxylic acid and alkyl azides)

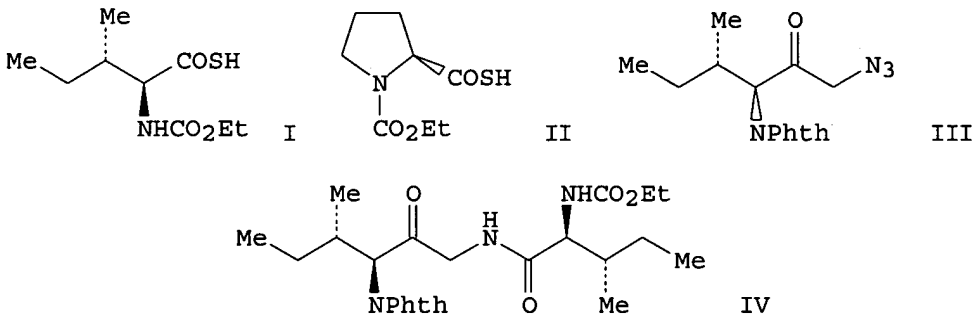
RN 98-91-9 HCAPLUS
CN Benzenecarbothioic acid (9CI) (CA INDEX NAME)



RN 507-09-5 HCAPLUS
CN Ethanethioic acid (9CI) (CA INDEX NAME)



L63 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:255276 HCAPLUS
DN 118:255276
ED Entered STN: 26 Jun 1993
TI Reductive acylation of α-keto azides derived from L-amino acids using N-protected L-aminothiocarboxylic S-acids
AU McKervey, M. Anthony; O'Sullivan, Michael B.; Myers, Peter L.; Green, Richard H.
CS Sch. Chem., Queen's Univ., Belfast, BT9 5AG, UK
SO Journal of the Chemical Society, Chemical Communications (1993), (1), 94-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
CC 34-2 (Amino Acids, Peptides, and Proteins)
OS CASREACT 118:255276
GI



AB Several homochiral N-protected α-amino carboxylic S-acids, e.g. I and II, have been synthesized from natural amino acids and used for reductive acylation of homochiral α,α'-amino keto azides, e.g. III (Pht = phthaloyl), also derived from natural amino acids. Thus, the reductive acylation of III with I gave 72% amide IV.
ST reductive acylation keto azide aminothiocarboxylic acid; thio amino acid reductive acylation
IT Reduction
(acylation and, of amino keto azides with protected thioamino acids)
IT **Azides**

RL: RCT (Reactant); RACT (Reactant or reagent)
(keto, reductive acylation of, with protected thioamino acids)
IT **Amides, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(amino, preparation of, by reductive acylation of amino keto azides with protected thioamino acids)
IT Acylation
(reductive, of amino keto azides with protected thioamino acids)
IT Amino acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(thio-, reductive acylation by, of amino keto azides)
IT 2419-38-7 3160-59-6 5123-55-7 29588-88-3
RL: PROC (Process)
(conversion of, to diazo ketone)
IT 1161-13-3 5700-74-3 5700-77-6 13734-34-4 16639-86-4 19887-31-1 122389-46-2
RL: PROC (Process)
(conversion of, to **thio acid**)
IT 28116-94-1P 96813-23-9P 114715-76-3P 147224-26-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to keto azide)
IT 92507-06-7P 147224-23-5P 147224-24-6P 147255-21-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyl azide)
IT 81000-39-7P 147224-21-3P 147224-22-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive acylation by, of amino keto azides)
IT 147224-27-9P 147224-28-0P 147224-29-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive acylation of, with protected thioamino acids)
IT 21171-97-1P 84235-32-5P 147224-25-7P 147224-30-4P 147224-35-9P 147224-36-0P 147224-37-1P 147255-22-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 147224-31-5P 147224-32-6P 147224-33-7P 147224-34-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by reductive acylation of amino keto azide with protected thioamino acid)
IT 622-79-7, Benzyl azide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with protected thioamino acids)

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(FILE 'CASREACT' ENTERED AT 09:29:39 ON 02 MAY 2005)

FILE 'CASREACT' ENTERED AT 09:30:35 ON 02 MAY 2005

FILE 'HCAPLUS' ENTERED AT 09:30:59 ON 02 MAY 2005
E AZIDE/CT
L48 21244 S E4,E5+OLD,NT,PFT,RT
E E3+ALL
L49 35908 S E3,E11+NT
L50 35912 S L48,L49
E AZIDE/CW
L51 35967 S E3,E4,L50
E AMIDE/CT
L52 173 S L51 AND AMIDE?/CW,CT
L53 3 S L52 AND (THIO OR THIOACETIC OR THIOBENZOIC)()ACID

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L54           0 S L52 AND (THIOACETATE OR THIOBENZOATE)
L55           4 S L52 AND L6,L7,L12
L56           5 S L53,L55
                E THIO/CT
                E E4+ALL
L57           4 S L52 AND E2
L58           6 S L56,L57
                E WILLIAMS L/AU
L59         101 S E3,E24,E25
                E WILLIAMS LARRY/AU
L60          15 S E3,E9
L61          39 S E47,E55,E56
L62           1 S L52 AND L59-L61
L63           6 S L58,L62

     FILE 'HCAPLUS' ENTERED AT 09:35:23 ON 02 MAY 2005

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=> fil casreact